

Isoamyl ether
544-01-4 | DTXSID8052198

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 177 °C

Global applicability domain: Inside

Local applicability domain index: 7.60e-01

Confidence level: 9.14e-01

Nearest Neighbors from the Training Set

Image not found

Isoamyl ether

Measured: 173

Predicted: 177

Image not found

Pentyl ether

Measured: 190

Predicted: 188

Image not found

Decane, 1-fluoro-

Measured: 186

Predicted: 185